and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ cannot have more than about one-tenth of the contribution of free O_2 molecules (Van Vleck, 1932) to the magnetic susceptibility of β-O_2. Magnetic and crystallographic studies of dilute solutions of O_2 in β-F_2 or in β-N_2 would be of interest in elucidating the disorder and interactions.

Table 1. *Structure factors for* β-F_2 and γ-O_2

	β–F_2		γ–O_2	
hkl	F_o	F_c	F_o	F_c
110	—	1·8	—	1·8
200	20·3	17·4	34·7	34·8
210	23·2	22·9	37·1	40·9
211	22·2	21·2	36·8	38·4
220	5·4	−5·7	9·9	−7·5
310	2·0	2·2	4·9	3·3
222	6·0	−2·6	17·9	−13·5
320	3·4	−1·6	13·9	−9·9
321	3·7	3·5	13·7	12·4
400	7·4	7·2	20·9	22·7
410	6·0	−5·5	12·2	−10·3
411	3·1	−4·1	7·3	−7·2
330	3·6	3·2	8·4	5·3
420	2·2	1·2	10·6	7·4
421	2·3	1·9	9·4	8·0
332	1·7	1·1	4·4	1·7
422	3·5	3·1	7·9	7·2
430	2·5	−3·0	6·3	−7·0
510	—	−0·8	—	0·1
431	1·7	−0·5	4·2	−1·8
520	1·9	0·8	4·2	1·6
432	2·0	1·7	—	1·3
521	1·3	−0·8	—	−0·5
440	2·5	−1·5	—	−0·9
530	1·3	0·9	—	2·9
433	—	0·7	—	1·2
531	—	0·0	—	0·0
600	2·1	−2·1	7·8	−7·3
442	2·1	0·3	1·7	2·8
610	—	1·3	—	4·4
611	—	0·1	4·4	2·5
532	1·7	−1·0	—	−2·7
620	1·9	−1·8	4·1	−6·0
621	—	0·4	4·3	−3·2
540	—	1·0	—	3·6
541	—	0·1	—	0·1
622	—	−0·2	—	−0·6
630	—	−0·2	—	−0·4
542	—	−1·0	—	−4·0
631	—	−0·1	—	0·6
444	2·6	−1·7	4·1	−6·3
632	—	0·3	2·9	2·4

The agreement obtained so far is about equally good for (*a*) spherically disordered O_2 (or F_2) at 000 and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ and cylindrically disordered O_2 in the other sites so that the bond lies in the plane of disorder ($R=0{\cdot}16$), and (*b*) a statistical model in which the F atoms of the molecular twofold site are in 16-fold positions ($\frac{1}{4}$ F's on threefold axes), and the F atoms of the other molecules are in 24-fold positions ($\frac{1}{2}$ F's in the plane of disorder). Large isotropic temperature factors are also required for model (*b*), which also yields $R=0{\cdot}16$ for either γ-O_2 or β-F_2 (Table 1). Three-dimensional electron density maps also indicate spherical disorder for the O_2's (F_2's) at 000 and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, but oblate spheroidal distributions for the other O_2's. Further studies of the many related types of disorder are in progress.

Note added in proof.— Later refinements have reduced R to 0·10 for β-F_2 and 0·13 for γ-O_2.

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References

Hu, J. H., White, D. & Johnston, H. L. (1953). *J. Amer. Chem. Soc.* **75**, 5642.

Kanda, E., Haseda, T. & Otsubo, A. (1955). *Science Reports of the Research Institutes, Tohoku Univ.* A–Vol. 7, No. 1, Sendai, Japan, Feb., 1955.

Knobler, C. M. (1961). Ph.D. Thesis, Leiden. 's-Gravenhage: Drukkerij Pasmans.

Lewis, G. N. (1924). *J. Amer. Chem. Soc.* **46**, 2027.

Lien, W. H. & Phillips, N. E. (1961). *J. Chem. Phys.* **34**, 1073.

Murphy, G. M. & Rubin, E. (1952). *J. Chem. Phys.* **20**, 1179.

Pauling, L. (1960). *The Nature of the Chemical Bond.* Cornell Univ. Press, 3rd Edition, p. 354.

Ruhemann, M. (1932). *Z. Phys.* **76**, 368.

Streib, W. E. & Lipscomb, W. N. (1962). *Proc. Nat. Acad. Sci. U.S.* **48**, 911.

Streib, W. E., Jordan, T. H. & Lipscomb, W. N. (1962). *J. Chem. Phys.* **37**, 2962.

Van Vleck, J. H. (1932). *The Theory of Electric and Magnetic Susceptibilities*, p. 266. Oxford Univ. Press.

Vegard, L. (1935*a*). *Nature, Lond.* **136**, 720.

Vegard, L. (1935*b*). *Z. Phys.* **98**, 1.

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On the symmetry of phases in the reciprocal lattice: a simple method.

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No mention is made in recent papers on reciprocal lattice symmetry (Bienenstock & Ewald, 1962; Jeffery, 1963) of the technique of structure factor algebra to find phase relations between structure factors. Our simple 'do-it-yourself method' uses the information already contained in *International Tables for X-ray Crystallography* (1952). We only require the knowledge of the so called general positions which is equivalent to the knowledge of the symmetry elements. Indeed *to every symmetry operation* $\mathbf{r}\rightarrow\mathbf{r}'$ *corresponds a phase relation in reciprocal space.*

Let us illustrate the structure factor algebra method by the example of space group $P4_322$ (D_4^7) No. 95 where

the general position is $\pm(x, y, z;\ \bar{x}, \bar{y}, \frac{1}{2}+z;\ \bar{y}, x, \frac{3}{4}+z;\ y, \bar{x}, \frac{1}{4}+z)$ and let us find the phase relation corresponding to the symmetry operation $\mathbf{r}(xyz) \rightarrow \mathbf{r}'(\bar{y}, x, \frac{3}{4}+z)$.

This is done in four steps.

(1) Form the scalar product
$\mathbf{h}.\mathbf{r}' = h(\bar{y}) + kx + l(\frac{3}{4}+z)$.

(2) Isolate the translational component which gives rise to a phase factor $a = \exp 2\pi i\frac{3}{4}l = \exp(3\pi il/2)$.

(3) Rewrite the resting scalar product in the form $\mathbf{r}.\mathbf{h}' = xk + y(\bar{h}) + zl$, *i.e.* bring xyz into their usual sequence.

(4) The desired symmetry relation between structure factors is
$F(\mathbf{h}) = aF(\mathbf{h}')$, *i.e.*
$F(hkl) = \exp(3\pi il/2)F(k\bar{h}l)$.

If the reader is able to show that to the points $\mathbf{r}(xyz)$ and $\mathbf{r}'(\frac{1}{4}-z, \frac{1}{4}-y, x)$ of group $Fd3m(O_h^7)$ No. 227 corresponds the phase relation $F(hkl) = F(l\bar{k}\bar{h})\exp(\pi i(h+k)/2)$ he will probably have understood how to use the method.

The theoretical proof may be found in French (Bertaut, 1959), in English (Bertaut & Waser, 1957) and in German (Bertaut, 1958).

In Jeffery's (1963) notation, the phase relation under (4) reads

$$\alpha_{hkl} = \alpha_{k\bar{h}l} + (3\pi/2)\,l$$

whereas Jeffery writes

$$\alpha_{hkl} = \alpha_{\bar{k}hl} + (3\pi/2)\,l\,.$$

We must conclude and have checked that in Tables 1 and 2 given by Jeffery, $\alpha_{\bar{k}hl}$ should be replaced by $\alpha_{k\bar{h}l}$ and, *vice versa*, $\alpha_{k\bar{h}l}$ should be replaced by $\alpha_{\bar{k}hl}$.

Finally let us mention that all phase relations for centrosymmetric groups are given in *Tables de Linéarisation des Facteurs de Structure* (Bertaut & Dulac, 1955, 1956).

References

Bertaut, E. F. (1958). *Fortschr. Min.*, **36**, 119.

Bertaut, E. F. (1959). *Acta Cryst.* **12**, 541.

Bertaut, E. F., Dulac, J. (1955). *Tables de Linéarisation des Produits et Puissances des Facteurs de Structure. Grenoble, Laboratoire d'Electrostatique et de Physique du Métal.*

Bertaut, E. F. & Dulac, J. (1956). *Acta Cryst.* **9**, 322.

Bertaut, E. F. & Waser, J. (1957). *Acta Cryst.* **10**, 606.

Bienenstock, A. & Ewald, P. P. (1962). *Acta Cryst.* **15**, 1253.

Jeffery, J. W. (1963). *Acta Cryst.* **16**, 1239.

International Tables for X-ray Crystallography (1952). Vol. I. Birmingham: Kynoch Press.

Acta Cryst. (1964). **17**, 779

Lattice constants of some double sulphates $M_2Co(SO_4)_2.6H_2O$.

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The lattice constants of four isomorphous cobalt double sulphates $M_2Co(SO_4)_26H_2O$, with M = K, Rb, NH_4 and Cs, have been determined from powder X-ray photographs with a quadruple Guinier—de Wolff camera (de Wolff, 1948) and Cu $K\alpha$ radiation. Because of the larger deviations on the two outer strips, only the inner ones were used, one recording the powder lines of the cobalt double sulphate, the other recording the lines of a reference substance for which we chose potassium aluminum alum. In a separate measurement on a Debye-Scherrer X-ray photograph taken in a cylindrical camera with 9 cm diameter the unit cell edge of the potassium aluminum alum was found to be $12{\cdot}157_8$ Å, in excellent agreement with the value $12{\cdot}158 \pm 0{\cdot}001$ Å found by Klug & Alexander (1940).

Calibration of each film was based on this value of the alum unit cell edge. The measured line positions appeared to be, within the limits of errors, a linear function of the calculated positions.

Irregular deviations as found by Fisher (1957) were not observed.

With this linear function the line positions of the sulphates were corrected and the constants in the relation

$$\sin^2\theta = Ah^2 + Bk^2 + Cl^2 + Dhl$$

were calculated. B was found from $\sin^2\theta$ differences between hk_1l and hk_2l reflexions, A from $hk0$ reflexions, C from $0kl$ reflexions and from $\sin^2\theta$ differences between hkl and $\bar{h}kl$ reflexions and D from all hkl reflexions. Table 1 gives the calculated lattice constants with the standard deviation of the mean. The morphological axial ratios were taken from Groth (1908).

Table 1. *Lattice constants of* $M_2Co(SO_4)_2.6H_2O$

	K	Rb	NH_4	Cs
a_0	$9{\cdot}061 \pm 0{\cdot}003$ Å	$9{\cdot}180 \pm 0{\cdot}001$ Å	$9{\cdot}247 \pm 0{\cdot}001$ Å	$9{\cdot}316 \pm 0{\cdot}001$ Å
b_0	$12{\cdot}207 \pm 0{\cdot}001$	$12{\cdot}433 \pm 0{\cdot}001$	$12{\cdot}519 \pm 0{\cdot}001$	$12{\cdot}824 \pm 0{\cdot}001$
c_0	$6{\cdot}151 \pm 0{\cdot}002$	$6{\cdot}230 \pm 0{\cdot}003$	$6{\cdot}239 \pm 0{\cdot}001$	$6{\cdot}365 \pm 0{\cdot}002$
β	104° 48′ ± 2′	106° 01′ ± 1′	107° 02′ ± 1′	107° 07′ ± 1′
β (morph.)	104° 55′	106° 01′	106° 56′	107° 08′
Axial ratio	0·7423:1:0·5039	0·7384:1:0·5011	0·7386:1:0·4984	0·7265:1:0·4963
Axial ratio (morph.)	0·7404:1:0·5037	0·7391:1:0·5011	0·7392:1:0·4985	0·7270:1:0·4968